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Overview of Multifluid-Flow-Calculation Methods*+

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INTRODUCTION

Multiphase flow modelling (not to mention single-phase fluid flow) can involve any or several of a number of basic physical flow phenomena. Although there may be numerical methods for multiphase flow which can in principle treat all types of flow that might occur; the diversity of real flows makes it almost necessary to adapt numerical techniques to the physics of interest. Thus, for example, there are special methods for computing boundary layer flows, and quite different methods which efficiently describe vortex shedding in turbulent flow. In this survey I would like to discuss two categories of numerical methods which may be useful in multiphase flow research. The first category includes methods which are specifically intended for accurate computation of discontinuities and shocks, while the second category includes methods for smooth, subsonic flows in which compressibility plays a lesser role or is negligible.

In terms of the applications being discussed in this workshop, the first group of methods might be of interest in rocket exhaust plumes which certainly contain shocks. They could also be useful in interior ballistics: even though the goal of interior ballistics cycle analysis is essentially to avoid conditions which create shock waves, the computation method must be capable of recognizing these conditions in order to understand how to avoid them.

The methods I will discuss in the subsonic flow category might be of interest for frazil ice flows. These same methods could in fact also be applied to interior ballistics, but this would be inappropriate: much of the effort in developing the smooth flow methods has been directed at conditions which do not obtain in a gun barrel, whereas little effort has gone into accurately representing shocks. It would be equally inappropriate to apply these methods directly to rocket exhaust problems, although the lessons learned for smooth flows might be helpful in a limited way, for example in developing self-adapting schemes for partly shock-free regions.

METHODS FOR RESOLVING SHOCKS

There has been a good deal of recent research into computing techniques for shocks and discontinuities in single-phase flow. Since the emphasis in this workshop is on multidimensional multiphase flow, I will omit mention of some single-phase techniques which at present look difficult to generalize and discuss four methods for resolving shocks: the method of characteristics, the Particle-in-Cell technique (PIC), flux corrected transport, and random choice methods.

METHOD OF CHARACTERISTICS

The mathematical theory of characteristics is basic to the understanding of partial differential equations, particularly of hyperbolic type [1]. The theory can also be used as the basis of a numerical method for solving initial-boundary value problems for unsteady as well as boundary value problems for steady flows. Although one can allow the characteristics themselves to determine grid points as one moves away from the initial values, it is often found advantageous to adapt the method of characteristics to compute on a specified grid with fixed space modes and time levels. Even so, the determination of bicharacteristics in two space dimensions for unsteady flow can be quite cumbersome. Furthermore, practice has shown that when method-of-characteristics schemes are modified to be implicit, or to scrupulously conserve mass, for example, the end result looks very much like a finite difference method. Therefore, although characteristics are important to understanding the basic properties of flow equations, they are usually not an efficient way to approach numerical solution.

There is another reason why the method of characteristics may be unsuited for multiphase flow calculation. Some of the equation sets which are widely used to describe multiphase flow are in fact not hyperbolic. This means that there are not a sufficient number of real characteristic directions to guarantee that a solution can be obtained by the method of characteristics. It also turns out that these multiphase equation sets, when used to formulate an apparently natural initial-boundary value problem, result in a non-well-posed or ill-posed problem. This is a mathematical term which means (in this case) that the solution of the problem does not depend continuously on the data which specify it; any uncertainity in the data could produce uncontrollable fluctuations in the solution. It used to be thought that an ill-posed problem was inherently suspect and unsuitable for use in physical applications. However, in the last twenty years there has been a growing body of mathematical theory (e.g. [2]) which suggests that ill-posedness may often be the result of a poor interpretation of the words "depends continuously on"; by choosing function spaces very carefully, an ill-posed problem can often be transformed into a well-posed problem. A full mathematical theory of ill-posed multiphase flow equations has not been developed, but experience shows that they can give useful results in practice. I will return to this question later. In any case, if a non-hyperbolic equation set is used, the method of characteristics is not applicable.

PARTICLE-IN-CELL METHOD

This method was developed originally at Los Alamos for single-phase flow and has recently been extended to multiphase

flow calculations. In fact, it is the only method I am discussing under the shock category which has already been proved for multiphase flow. The example presented in the original communication [3] on this method was the impinging of a shock wave in a gas on a plate of fragmented metal. The authors claimed the PIC multifluid method preserved the shock profile much better than simple finite difference schemes.

The basis idea of the particle-in-cell method is that, in addition to a standard space mesh with each cell having values of fluid properties (e.g., pressure, temperature, velocity) ascribed to it, there are also a number of marker particles in each cell. These marker particles are used in an essential way to solve unsteady flow equations. The procedure is essentially the following.

At the beginning of a calculation, particles are assigned to coordinate locations in all the cells and distributed proportionally to the initial fluid densities. Separate particles are defined for each phase, and they are given the fluid properties of the cell in which they start. To advance the calculation one time step, one first computes changes in the Eulerian variables for each cell due to all phenomena except convection (and thermal conduction). In other words, the equations of motion are solved as if they were Lagrangian. In the second stage, the marker particles are used. The motion of each particle is computed; from the displacements one sees which particles have crossed Eulerian cell boundaries. These movements are used to adjust the mass, momentum, and energy of each Eulerian cell, and this is the means by which the effect of convection is computed. In a final stage, the conduction of heat is determined.

This method appears to be an effective way of resolving shocks without using an extremely fine Eulerian mesh. The disadvantage of the method is the computing overhead associated with the particles, of which there must be several per mesh cell. This overhead may be less of a burden in multiphase flow (which already requires complex equation sets) than in single-phase flow; but it may be more of a burden in multidimensional calculations than in one dimension. For these reasons we will discuss two other numerical methods which, although apparently not yet tested for multiphase flow applications, do show considerable promise.

One final remark on the particle-in-cell method: in the interior ballistics problem for charges with large chunks of prismatic solid propellant, there is a very natural way to choose marker particles. With coarse propellant particles, only a few marker particles per mesh cell would be required. A modified PIC method might be valuable where marker particles have a natural physical meaning and can be described in special detail.

FLUX-CORRECTED TRANSPORT

Finite difference methods typically behave in one of two ways when applied to discontinuities. Low order schemes tend to smear distontinuities, so that a sharp local jump in flow variables becomes a sloping change over several mesh cells. High order schemes give steeper, more localized jumps, but as a side-effect they create ringing oscillations on either side of the jump, similar to the Gibbs phenomenon in Fourier series analysis. The basic difficulty is that low vs. high order of approximation is a concept applicable to curves with a certain degree of smoothness, but not very useful for curves with jump discontinuities. Something more than just a higher order approximation is needed to treat shocks.

Flux-corrected transport is a technique which can be applied to a variety of finite-difference schemes, and offers a way around the low vs. high order dilemma. The idea of the method can be seen by considering the simple continuity equation:

$$\partial\rho/\partial t = -\nabla \cdot (\rho v)$$

The flux-corrected transport procedure falls into two stages. The first is a transport phase in which one solves finite difference equations such as

$$\bar{\rho}_j = \rho_j^n - \tfrac{1}{2}\varepsilon\Delta_j\rho^n + (\tfrac{1}{8} + \tfrac{\varepsilon^2}{2})\,\Delta_j^2\,\rho^n ,$$

where the parameter $\varepsilon = v\,\Delta t/\Delta x$ has been introduced. The 1/8 term introduces a diffusion of mass which is velocity-independent. The basic point is that the first stage be a low-order scheme which is positive (i.e., causes enough smearing to guarantee that no ripples are created).

The second, or anti-diffusion, stage then attempts to compensate for this smearing. Schematically we can write the second stage equation

$$\rho_j^{n+1} = \bar{\rho}_j - \text{"}\tfrac{1}{8}\;\Delta_j^2\,\bar{\rho}\text{"}$$

The quote marks indicate that what we have written needs clarification. In fact, the second difference of $\bar{\rho}$ is represented by a first difference of mass fluxes $f_{j+1/2}$ and $f_{j-1/2}$.

By observing that these fluxes can be individually adjusted without damaging the conservative property of the difference procedure, we are freed for the essential trick: these fluxes are adjusted so that no new extrema are produced in the solution. Doing this carefully will therefore reduce smearing without producing Gibbs overshoot.

The above description of flux-corrected transport has been cribbed from the original paper by Boris and Book [4]. Flux-corrected transport has gained a reputation as a technique which

works well in practical computation. Modifications and extensions have been proposed; see for example [5]. An important question, for these or other modifications of finite difference methods, is to what extent they are truly shock-capturing techniques, in other words, whether they contain concealed topological tests which are used to identify shock fronts (as shock tracking methods frankly do). The danger of such hidden topological content is that complex or unexpected shock patterns arising from real problems (e.g. [6]) may not conform to what the numerical method expects. For this reason, considerable care is needed, and evaluation based on simple test problems [7], although helpful, is not necessarily conclusive.

RANDOM CHOICE METHODS

Random choice methods originated in a proof by Glimm of the existence of solutions to certain nonlinear hyperbolic systems of equations. The original random choice method was distinctly not a finite difference method. The basic idea involved the use of Riemann solutions, i.e., solutions to the compressible flow equations on an infinite domain with one constant initial state on the left and another constant initial state on the right. (The original random choice method was conceived in one space dimension.) Riemann soltuions can be constructed if the two states are specified; in general they are composed of a rarefaction wave, a contact discontinuity, and a shock all emanating from the point of which the two constant initial states touched.

The random choice method utilizes these Riemann solutions in the following way. At time t_o the space domain is divided into intervals and the solution at t_o is approximated by a piecewise constant function with a step jump in each interval. Within each interval, the solution of the corresponding Riemann problem is evaluated. This Riemann solution is advanced to

$t_o + \Delta t$, where a random sample of the Riemann solution is

taken. The sample values in the various intervals define a new piecewise constant function which approximates the solution of the flow equations at $t_o + \Delta t$.

This approximation procedure converges to a solution of the initial value problem if the initial values are nearly constant, which leads to Glimm's existence result. In its original form, however, the method was not effective as a practical numerical scheme. Somewhat later, Chorin [8] refined the method, in particular the random sampling procedure, and showed that random choice methods could be competitive for practical calculations. Since they take specific account of discontinuities, it is not too surprising that they can, for example, propagate shocks with no distortion. They also seem to perform well in realistic, complicated problems.

One limitation of the original random choice method is the fact that it is not easy to generalize to more than one space dimension. One way to get around this problem is to use a locally one-dimensional, or time-splitting approach, where each time step is split into a fractional step solving the terms with derivatives in one space direction, followed by a fractional step solving in the orthogonal direction. This approach works, but has difficulty describing a discontinuity which propagates obliquely to the coordinate axies. Remedies for this may include use of special coordinate grids, or shock-tracking procedures, but they typically presuppose some knowledge of the topology of the discontinuities which may appear. Again, this type of assumption has its dangers when carried over to applications where the topology of shocks is complex or not know in advance.

Very recently, Peter Lax and A. Harten have proposed a substantial modification of random choice methods which is a random choice finite difference method [9]. By replacing the Riemann solution with a finite difference solution, two important paths are opened: the method may be applicable to more complicated equations, such as multiphase flow systems, where the Riemann problem cannot readily be solved in closed form; and a truly multidimensional approach may become feasible.

METHODS FOR SUBSONIC FLOW

The methods to be discussed below are perhaps misrepresented by describing them as subsonic flow methods; more precisely, they are methods which have been devised with a view toward computing with large time step sizes. This means that they are suited to transients in which the timescales of interest are large compared with the time required for a disturbance travelling at sonic velocity to traverse the space region of interest. Thus they are appropriate for problems with smooth flow conditions which evolve relatively slowly. As mentioned above, it does not necessarily mena that they are incapable of describing shocks: they can, but not as well as methods devised for that purpose. The methods below could be modifified or adapted to compute shock problems. But if a principle feature of the problem is to investigate in detail the propagation of perturbations (especially shocks) at sonic or supersonic speeds, then it is unlikely that the effort devoted to allowing large time step sizes would be used advantageously.

FRACTIONAL STEP METHODS

One general and useful approach which helps to allow computing with larger time step sizes is the method of fractional steps, first discussed in a systematic way by Yanenko [10]. There are many variants of the method of fractional steps, most of them aimed at implicit time-difference treatment of complex

problems. If an evolution equation splits into two parts,

$$\phi_t + A\phi + B\phi = 0,$$

where the simpler equations $\phi_t + A\phi = 0$ and $\phi_t + B\phi = 0$ can be solved readily with stable implicit differences, then a fractional step method

$$(\phi^{n+1/2} - \phi^n)/\Delta t + A\phi^{n+1/2} = 0$$
$$(\phi^{n+1} - \phi^{n+1/2})/\Delta t + B\phi^{n+1} = 0$$

can be used to obtain a numerically stable scheme for the original equation. It should be noted that "$n+1/2$" does not refer to a time between levels n and n+1; it indicates an intermediate result used to arrive at level n+1. That the fractional step method above (also called a time-splitting method) yields a solution of the original equations can be seen by adding the two difference equations. The overall method in this case is stable if each step by itself is stable.

The splitting of the evolution operator into parts A and B may be done in any way which is convenient and appropriate to the problem at hand. Many fractional step methods have been based on time-splitting by space direction, as mentioned above under random choice schemes. Another possibility is splitting by physical phenomenon. An example of this approach will be discussed below.

Locally one-dimensional techniques, or time-splitting based on space direction, have been used by various authors, for example [11], in single-phase flow calculation to achieve large time step sizes. Applications include supersonic flow with shocks, but more often for steady flow calculation. Locally one-dimensional techniques are susceptible to errors or inefficiency in following disturbances which move obliquely to the coordinate axes. This problem has been found more severe with less compressible fluids, which is the main reason that other techniques are being developed for applications like bubbly two-phase flow.

SEMI-IMPLICIT METHOD

The semi-implicit method of Liles, Reed, and Mahaffy [12], [13] is currently the most coherent numerical technique for smooth two-phase flows. It is an extension of the ICE method [14] and the IMF [15] technique of Harlow and Amsden. There is a basic philosphy behind the method, closely tied to the physics of flows. For reference, the two-fluid flow equations solved are the equations of mass, momentum, and energy conservation for each phase:

$$\partial \alpha \rho_v / \partial t + \nabla \cdot \alpha \rho_v \underline{v}_v = \Gamma$$

$$\partial (1-\alpha) \rho_\ell / \partial t + \nabla \cdot (1-\alpha) \rho_\ell \underline{v}_\ell = -\Gamma$$

$$\alpha \rho_v [\partial \underline{v}/\partial t + \underline{v}_v \cdot \nabla \underline{v}_v] + \alpha \nabla P = -K(\underline{v}_v - \underline{v}_\ell) - \underline{F}_v \cdot \underline{v}_v - \underline{g}_v$$

$$(1-\alpha) \rho_\ell [\partial \underline{v}_\ell / \partial t + \underline{v}_\ell \cdot \nabla \underline{v}_\ell] + (1-\alpha) \nabla P = K(\underline{v}_v - \underline{v}_\ell) - \underline{F}_\ell \cdot \underline{v}_\ell - \underline{g}_\ell$$

$$\partial \alpha \rho_v e_v / \partial t + \nabla \cdot \alpha \rho_v e_v \underline{v}_v + P[\partial \alpha / \partial t + \nabla \cdot \alpha \underline{v}_v] = Q + Q_v$$

$$\partial (1-\alpha) \rho_\ell e_\ell / \partial t + \nabla \cdot (1-\alpha) \rho_\ell e_\ell \underline{v}_\ell + P [-\partial \alpha / \partial t + \nabla \cdot (1-\alpha) \underline{v}_\ell] = -Q + Q_\ell$$

The goal of the semi-implicit technique is to solve difference equations which are as implicit as possible and still permit an efficient and robust method of solving for the new time unknowns at each time step. If we categorize the physical phenomena in the above equations as interphase exchanges, sonic propagation, and fluid convection, then the semi-implicit method treats the first two (which typically have short time scales) implicitly, while convection (having a somewhat longer time scale) is treated explicitly. It turns out that if difference equations are written which follow this philosphy, then the coupling of new-time unknowns in the difference equations has a relatively simple structure.

The unknowns are found by a two-level procedure. First, the equations are linearized about some guessed value of the unknowns. (After the linearized equations are solved, the linearization is repeated, so the outer level amounts to Newton's method for solving the nonlinear semi-implicit difference equations). Then the linearized equations are solved, by first carrying out a local reduction of the system of equations. For each cell, the unknown velocities, and then the void fraction and temperatures can be eliminated by simple manipulation of difference equations around that cell only. This reduction is not only rapid, but leads to a set of equations for the pressures only, having important properties.

The pressure equations represent, in compact form, the fully coupled effects of sonic propagation and interphase coupling over the time step. In addition, they can be shown to form a system of Poisson type. This means that any of a number of standard direct or iterative methods with well-understood properties can be used to solve the pressure problem. Once pressures are found, the other unknown are deduced from the pressures.

In summary, the semi-implicit method is based on a systematic physically-based choice of difference equations, which can then be solved by a combination of well-understood techniques. The mathematical theory behind these techniques guarantees the convergence of the iterations involved, and makes for a method which in practice is exceptionally robust. Because

the difficult coupling of unknowns is reduced to a simple Poisson problem, the basic method is probably as efficient as possible for the chosen degree of implicitness. A large number of multi-dimensional two-phase flow problems in nuclear reactor safety have been solved using this method in the TRAC [16] and THERMIT [17] codes. A detailed description of the method can be found in [17].

We mentioned above that some two-fluid models of two-phase flow are ill-posed in the mathematical sense; the equations displayed above are one such ill-posed system. To understand why practical calculations show no evidence of ill-posedness, a stability analysis of the semi-implicit method for the two-fluid model was carried out [18]. Briefly, it was found that interfacial drag acts as a damping term, so that if the mesh size is not too small, solutions to the difference equations should be well-behaved. Furthermore, there are physically understandable constraints on the minimum mesh size: for example, in bubbly flow the mesh should not be finer than the size of an individual bubble. This analysis is somewhat reassuring, but open questions remain and a more rigorous theory (or an improved physical model) is needed.

METHODS TREATING CONVECTION IMPLICITLY

While the semi-implicit method is very effective for many transient calculations, there are still some problems where significant physical changes in the flow occur only on a rather long time scale. Since the semi-implicit method treats convection explicitly, time steps may be longer than the least time taken for fluid to travel from one cell to the next. For some problems one would like to be able to take larger time steps, because the maximum semi-implicit time step size is small compared to the time for the flow to alter itself noticeably.

For problems which can be handled by one-dimensional calculation there is no great difficulty about using a fully implicit scheme. One can write fully implicit difference equations, linearize them about a guessed soltion and solve the linear system by Gaussian elimination. This is feasible because the bandwith in the one-dimensional case is no more than 6 unknowns × 3 nodes = 18. Such a method is equivalent to a method of lines. Refinements of this approach for two-fluid models are in use [19,20].

For multidimensional problems, however, such an approach would be far too costly for any but the smallest problems. Two alternatives are currently being pursued.

One involves fractional step methods. To avoid the risks of locally one-dimensional techniques, effort is focused on splitting by physical phenomena. This is one way to retain the benefits of the semi-implicit method. A recent paper [21] shows

how a stabilizing corrections method (which is one type of fractional step method) can be used to overcome the limitation on time step size due to convection in one coordinate direction. The basic idea is to perform a semi-implicit first fractional step (with Δt larger than the convection limit), and then in a second fractional step to recompute terms involving convection in one direction implicitly. The second step removes the destabilizing effects of having exceeded the limiting time step size in the first fractional step, hence the name stabilizing correction. This method has been shown to be advantageous for slowly evolving transient with flow velocities primarily along one coordinate axis.

If, as appears possible, this technique can be generalized, it should lead to a fractional step method which dispenses entirely with any upper limit on the time step size.

A second attack on the convection time step limit in multidimensional calculation is more frontal: fully implicit difference equations are written and solved by a clever iterative method. One such fully implicit method [22] is an outgrowth of an earlier fully implicit method for single-phase flow [23]. The single-phase method has recently been studied by Wachspress [24]; in particular, he gave a mathematical analysis which helps understand the choice of crucial underrelaxation parameters. For the corresponding two-phase method, it appears that underrelaxation parameters are also needed, and although even more skill is required in choosing these, there is as yet no basis in mathematical/physical analysis for doing this. Therefore the method cannot be considered robust, for even though someone who is skillful in choosing underrelaxation parameters may obtain good results with the method, there is no guarantee that another user (or the same user with a different problem) will not suddenly find things otherwise.

CONCLUSION

My purpose in this lecture has been to discuss some of the many numerical methods for fluid flow calculation which might be of interest for multiphase flow. The most effective and reliable numerical methods seem to be based on both clear understanding of relevant physics, and mathematical ideas which guarantee or make plausible the practical success of the methods. Some methods have come from mathematicians familiar with physical problems, while others have been devised by physicists or engineers who recognize the important mathematical principles. More complex and sophisticated applications will undoubtedly require continued appreciation of both facets.

References

1. R. Courant and D. Hilbert, "Methods of Mathematical Physics," Vol. II, Interscience, New York, 1962.

2. L.E. Payne, "Improperly Posed Problems in Partial Differential Equations," SIAM Regional Conference Series in Applied Mathematics, Philadelphia, 1975.

3. T.L. Cook, R.B. Demuth and F.H. Harlow, "PIC Calculations of Multiphase Flow," LA-UR-79-2956, 1979.

4. J. P. Boris and D.L. Book, J. Computational Physics 11, 38-69 (1973).

5. S.T. Zalesak, J. Computational Physics 31, 335-362 (1979).

6. D.L. Book, "Two Dimensional FCT Model of Low-Altidude Nuclear Effects," NRL Memorandum Report 4362, 1980.

7. G.A. Sod, J. Computational Physics 27, 1-31 (1979).

8. A.J. Chorin, J. Computational Physics 22, 517-533 (1976).

9. P.D. Lax and A. Harten, "A Random Choice Finite Difference Scheme for Hyperbolic Conservation Laws," to appear in SIAM J. Numerical Analysis.

10. N.N. Yanenko, "The Method of Fractional Steps," Springer-Verlag, New York-Heidelberg-Berlin, 1971.

11. R.F. Warming and R.M. Beam, "On the Construction and Application of Implicit Factored Schemes for Conservation Laws in Computational Fluid Dynamics," SIAM-AMS Proceedings, Vol. XI, Amer. Math. Soc., Providence, R.I. 1978.

12. D.R. Liles and Wm. H. Reed, J. Computational Physics 26, 390-407 (1978).

13. J. H. Mahaffy, in Report LA-7039-PR, 1977.

14. F.M. Harlow and A.A. Amsden, J. Computational Physics 8, 197-213 (1971).

15. F.J. Harlow and A.A. Amsden, J. Computational Physics 17, 19-52 (1975).

16. TRAC Reference Manual, Report LA-7279-MS, 1978.

17. W.H. Reed and H. B. Stewart, THERMIT Reference Manual, report prepared for EPRI under Contract RP-518.

18. H.B. Stewart, J. Computational Physics 33, 259-270 (1979).

19. J.H. Mahaffy, Report LA-7951-MS, 1979.

20. D.A. Dube, "Development of a fully implicit two-fluid thermal-hydraulic model for boiling water reactor transient analysis," Ph.D. thesis, Massachusetts Institute of Technology, 1980.

21. H.B. Stewart, J. Computational Physics 39, (1981).

22. D.B. Spalding, these Proceedings.

23. S.V. Patankar and D.B. Spalding, Int. J. Heat Mass Transfer 15, 1787 (1972).

24. E.L. Wachspress, Report KAPL-4116, 1979.